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UNPUBLISHED PRELIMINARY DATA

Oscillator Strengths and High Accuracy

Wave Functions for Neutral Helium\*†

Louis C. Green†, Eleanor K. Kolchin and

Norma C. Johnson

Strawbridge Observatory, Haverford College,

Haverford, Pa.

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## Abstract

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Oscillator strengths have been computed for the  $1^1S-n^1P$  series of HeI. The computations were carried through with wave functions determined by the minimum principle and employed central field functions and configuration interaction. The agreement between the oscillator strengths as computed by the length, velocity, and acceleration expressions and the agreement between the present work and the very extensive computations of Schiff and Pekeris for the transitions  $1^1S-2^1P$  and  $1^1S-3^1P$  give confidence in the effectiveness of the method and the dependability of the results.



### Introduction

For any relatively complete, quantitative interpretation of astronomical spectra, it is essential to have available the relevant transition probabilities. To obtain dependable transition probabilities theoretically, it is necessary to employ wave functions of considerable accuracy. This requirement follows from the sensitivity of the transition probabilities to the form of the wave function, particularly to the positions of the zeros.<sup>1,2,3,4</sup>

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<sup>1</sup> D.R. Bates, Proc. Roy. Soc., London, A, 188, 350 (1947).

<sup>2</sup> L.C. Green and N.E. Weber, Astrophys. J., 111, 582 (1950).

<sup>3</sup> A. Delgarno and N. Lynn, Proc. Phys. Soc. (London) A70, 802 (1957).

<sup>4</sup> A. Delgarno and A.E. Kingston, Proc. Phys. Soc. (London) 72, 1053 (1958).

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For two-electron atomic systems, it is well known that either of two closely related methods, that of Hylleraas, which employs the interelectron distance,  $r_{12}$ , and that of Pekeris, which employs perimetric coordinates, can give excellent results.<sup>5</sup>

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<sup>5</sup> L.C. Green, E.K. Kolchin and N.C. Johnson, Phys. Rev.

This paper gives numerous references to the earlier literature.

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Unfortunately neither of these procedures seems appropriate for more complex systems. In the case of the Hylleraas method, the number of  $r_{ij}$ 's increases rapidly with the number of electrons and the space must be repeatedly divided to deal with the integrals involving them. On the other hand, there is no known way of extending the method of perimetric coordinates to deal with three or more electrons.

In contrast, the experimental spectroscopists have had remarkable success in analyzing even the most complex spectra in the first approximation in terms of central field wave functions. The method of configuration interaction is available for carrying the treatment to a higher approximation. The present work is the result of the decision to push the configuration interaction approach further and to apply it to two-electron systems where its results can be compared with those from other methods. Among the two-electron spectra, HeI was chosen because of its astrophysical importance and because of the extent of the experimental information available.

### The Wave Functions

Regardless of which of the above methods is employed, one can use the energy integral and the minimum principle to choose the values of arbitrary parameters which have been introduced into the wave functions. In the present case, the trial variational function has been given the form,

$$\Psi_m = \sum_{k=L+1}^m c_k \Phi_k \quad (1)$$

Here  $n$  is the value of the principal quantum number of the running electron in whichever series of terms is being considered. For example, in the case of the  $4^3P$  term which arises from the  $1s4p$  configuration,  $n$  would be 4.  $L$  in Eq. (1) is the total orbital angular momentum quantum number for the series and the  $\Phi_k$ 's are defined by the equation,

$$\Phi_k = \sum_i c_{ki} \psi_i \quad (2)$$

where the  $\psi_i$ 's are linear combinations of normalized anti-symmetrized products of Slater orbitals. The orbitals are chosen so that  $M_S=0$  and  $M_L=0$  for each product. Clebsch-Gordon coefficients are employed to assign weights to these products such that their linear combinations have the correct spin and angular dependence for eigenfunctions in LS-coupling. The  $\psi_i$ 's therefore have the form,

$$\begin{aligned} \psi_i = \sum_{m_s} \left\{ C\left(\frac{1}{2}, \frac{1}{2}, S, m_s\right) \sum_{m_i=-\ell_i}^{\ell_i} \left[ C(\ell_i, \lambda_i, L, m_i) \cdot \right. \right. \\ \cdot N A \left\{ \lambda_1^{a_i} \exp\left(-Z \frac{\alpha_i}{\kappa \alpha_i} \lambda_1\right) Y(\ell_i, m_i; \theta_1, \varphi_1) \delta(m_s; \sigma_1) \cdot \right. \\ \left. \left. \lambda_2^{b_i} \exp\left(-Z \frac{\beta_i}{\kappa \beta_i} \lambda_2\right) Y(\lambda_i, -m_i; \theta_2, \varphi_2) \delta(-m_s; \sigma_2) \right\} \right\} \quad (3) \end{aligned}$$

Here  $\ell_i$  and  $\lambda_i$  are the orbital angular momentum quantum numbers of the two electrons with  $\ell_i \leq \lambda_i$ , the  $C$ 's are the Clebsch-Gordon coefficients,  $N$  is the normalization constant for the antisymmetrized product which follows,  $A$  is the antisymmetrizer operator, the  $Y$ 's are surface spherical harmonics and the  $\delta$ 's are Kroeneker deltas, employed here as spin functions.

The  $a_i$ 's and  $b_i$ 's are integers,  $Z$  is an arbitrary constant which is usually set equal to the nuclear charge, the  $n_{\alpha i}$ 's and  $n_{\beta i}$ 's are the principal quantum numbers of the two electrons, the  $\alpha_i$ 's and  $\beta_i$ 's measure the strength of the "effective nuclear charge" for each electron, that is, the nuclear charge minus the screening due to the other electron.

The adjustable parameters fall into two classes, those which enter the wave function linearly and those which do not. The  $c_k$ 's and  $c_{ki}$ 's are in the first class and  $a_i$ 's,  $b_i$ 's,  $\alpha_i$ 's and  $\beta_i$ 's in the second. One of the advantages of the method of configuration interaction is that the results of the experimental spectroscopists and physical intuition suggest initial trial values for the non-linear parameters. These initial values can then be refined rather quickly by trial and error or more systematic procedures.

For fixed values of the non-linear parameters, the conditions for a minimum yield in the case of the wave function for the lowest member of any series,  $\psi_{L+1}$ , the set of homogeneous linear equations,

$$\sum_j c_{i+1,j} (H_{ij} - N_{ij}\lambda) = 0 \quad (4)$$

where

$$H_{ij} = \int \psi_i^* H \psi_j d\tau \quad \text{and} \quad N_{ij} = \int \psi_i^* \psi_j d\tau \quad (5)$$

and  $\lambda$  is a Lagrangian multiplier which introduces the auxiliary condition that  $\psi_{L+1}$  is normalized. To obtain non-trivial values for the  $c_{ij}$ 's, one finds the lowest eigenvalue of  $\lambda$

~~is~~<sup>for</sup> the secular determinant

$$|H_{ij} - N_{ij}\lambda| = 0 \quad (6)$$

This eigenvalue is also the energy to be associated with the lowest term of the series.<sup>6</sup>

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<sup>6</sup> For a discussion of the application of variational methods to the determination of eigenvalues and eigenfunctions, see numerous textbooks on quantum mechanics; for example, L. Pauling and E.B. Wilson, Introduction to Quantum Mechanics (McGraw-Hill Book Co., Inc., New York, 1935).

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When sets of non-linear parameters have been found which give an energy satisfactorily close to the observed, the  $c_{L+1,j}$ 's are found and the whole  $\Phi_{L+1} = \Psi_{L+1}$  is frozen. For  $\Psi_{L+2}$ , one writes

$$\Psi_{L+2} = c_{L+1}\Phi_{L+1} + c_{L+2}\left(\sum_i c_{L+2,i}\psi_i\right) \quad (7)$$

The same procedures as before are now repeated with a new choice of non-linear parameters in the  $\psi_i$ 's and use of the second eigenvalue of the new secular determinant. The above process is continued until as many  $\Phi_k$ 's have been found as the number of terms which are being considered in the particular series.

$$\Psi_n = \sum_{k=L+1}^{n-1} c_k \Phi_k + c_n \left( \sum_i c_{ni} \psi_i \right) \quad (8)$$

If N is the value of n for the highest series member of interest, one may write

$$\Psi_n = \sum_{k=L+1}^N c_k \Phi_k \quad (9)$$

and, as a possible final step, one may find the first  $N$  eigenvalues of the associated  $(N-L) \times (N-L)$  secular determinant where the various  $\bar{\phi}_k$ 's are taken as fixed. Since it would be possible to use a wide variety of arbitrarily chosen functions for the  $\bar{\phi}_k$ 's, subject to only a rather small number of not very restrictive conditions, the whole calculation may be thought of as starting with Eq. (9) with the  $\bar{\phi}_k$ 's given. Nevertheless, in view of the way in which the  $\bar{\phi}_k$ 's were chosen, it is clear that the  $c_k$ 's for any  $k > n$  should be small. This in fact proves to be the case and indeed the energies as calculated with the wave functions of Eqs. (8) and (9) never differ by as much as  $1 \cdot 10^{-6}$  rydbergs, that is, by as much as  $0.1 \text{ cm}^{-1}$ .

The Expression for the Matrix Elements

More specifically,  $H_{ij}$  in Eq. (5) will be a sum of four terms in the general case. If we omit the Clebsch-Gordon coefficients, the spin factors and the normalization constant  $N$ , a typical member of these four terms will have the form

$$d = \int c_i \exp \left[ -Z \left( \frac{\alpha_i}{m \alpha_i} r_1 + \frac{\beta_i}{m \beta_i} r_2 \right) \right] r_1^{a_i} r_2^{b_i} Y^*(l_i, m_i; \theta_1, \phi_1) Y^*(l_i, -m_i; \theta_2, \phi_2) \cdot \\ \cdot H \left\{ c_j \exp \left[ -Z \left( \frac{\alpha_j}{m \alpha_j} r_1 + \frac{\beta_j}{m \beta_j} r_2 \right) \right] r_1^{a_j} r_2^{b_j} Y(l_j, m_j; \theta_1, \phi_1) Y(l_j, -m_j; \theta_2, \phi_2) \right\} dr$$

$$\text{where } H = - \left\{ \frac{\partial^2}{\partial r_1^2} + \frac{2M}{r_1} + \frac{1}{r_1^2} \left[ \frac{1}{\sin \theta_1} \frac{\partial}{\partial \theta_1} \left( \sin \theta_1 \frac{\partial}{\partial \theta_1} \right) + \frac{1}{\sin^2 \theta_1} \frac{\partial^2}{\partial \phi_1^2} \right] + \right. \quad (10)$$

$$\frac{\partial^2}{\partial r_2^2} + \frac{2M}{r_2} + \frac{1}{r_2^2} \left[ \frac{1}{\sin \theta_2} \frac{\partial}{\partial \theta_2} \left( \sin \theta_2 \frac{\partial}{\partial \theta_2} \right) + \frac{1}{\sin^2 \theta_2} \frac{\partial^2}{\partial \phi_2^2} \right] \\ \left. - 2 \sum_k \left[ \frac{\lambda_c^k}{\lambda_c^{k+1}} \frac{4\pi}{2k+1} \sum_{\mu=-k}^k Y(k, \mu; \theta_1, \phi_1) Y^*(k, \mu; \theta_2, \phi_2) \right] \right\} \quad (11)$$

and

$$d\tau = \sin \theta_1 d\theta_1 d\phi_1 dr_1 \sin \theta_2 d\theta_2 d\phi_2 dr_2 \quad (12)$$

In Eq. (11),  $M$  is the nuclear charge. It is to be noted that  $Z$  is arbitrary but is usually set equal to  $M$  while the choice of the  $\alpha$ 's and  $\beta$ 's for a wave function is being made. When the choice is made,  $Z$  may be varied to insure that the Virial Theorem is satisfied. In those cases in which this variation was actually made, the best value of  $Z$  was found to differ by ~~less~~ <sup>than</sup> 0.0001 from  $M$  and the energy was changed by less than 0.000001 rydbergs.

If we let  $x \equiv a_i + a_j$ ,  $y \equiv b_i + b_j$ ,  $u \equiv \alpha_i + \alpha_j$  and  $v \equiv \beta_i + \beta_j$ , the value of the integral in Eq. (10) may be written in the form

$$\begin{aligned}
 \mathcal{I} = & -\frac{c_i c_j}{z^{x+y+2}} \left[ \delta(l_i, l_j) \delta(m_i, m_j) \delta(\lambda_i, \lambda_j) \right. \\
 & \cdot z^2 \left\{ (\alpha_j^2 + \beta_j^2) \frac{x!}{u^{x+1}} \frac{y!}{v^{y+1}} - 2\alpha_j a_j \frac{(x-1)!}{u^x} \frac{y!}{v^{y+1}} + [a_j(a_j-1) - l_j(l_j+1)] \frac{(x-2)!}{u^{x-1}} \frac{y!}{v^{y+1}} \right. \\
 & \quad \left. - 2\beta_j b_j \frac{x!}{u^{x+1}} \frac{(y-1)!}{v^y} + [b_j(b_j-1) - \lambda_j(\lambda_j+1)] \frac{x!}{u^{x+1}} \frac{(y-2)!}{v^{y-1}} \right\} \\
 & + 2z \left\{ \delta(l_i, l_j) \delta(m_i, m_j) \delta(\lambda_i, \lambda_j) M \left[ \frac{(x-1)!}{u^x} \frac{y!}{v^{y+1}} + \frac{x!}{u^{x+1}} \frac{(y-1)!}{v^y} \right] \right. \\
 & \quad \left. - \sum_{k=k_{\min}}^{k_{\max}} \left[ c^k(l_i, m_i, l_j, m_j) c^k(\lambda_j, m_j, \lambda_i, m_i) \right. \right. \\
 & \quad \left. \left. \cdot \{ B(u, v, x-k-1, y+k) + B(v, u, y-k-1, x+k) \} \right] \right\}
 \end{aligned}$$

(13)

where  $k_{\min}$  is the larger of  $|l_i - l_j|$  and  $|\lambda_i - \lambda_j|$  and  $k_{\max}$  is the smaller of  $l_i + l_j$  and  $\lambda_i + \lambda_j$ . In Eq. (13), the  $c^k$ 's have the form <sup>7,8</sup>

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<sup>7</sup> E.U. Condon and G.H. Shortley, The Theory of Atomic Spectra (Cambridge University Press, London, 1935).

<sup>8</sup> J.C. Slater, Quantum Theory of Atomic Structure (McGraw-Hill Book Co. Inc., New York, 1960).

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$$c^k(l_i, m_i, l_j, m_j) = \sqrt{\frac{4\pi}{2k+1}} \int Y^*(l_i, m_i; \theta, \phi) Y(k, \mu; \theta, \phi) Y(l_j, m_j; \theta, \phi) \sin \theta d\theta d\phi \quad (14)$$

$$c^k(\ell_i, m_i, \ell_j, m_j) = (-1)^{m_i + \frac{1}{2}(|m_i| + |m_j| + |m_i - m_j|)}$$

$$\cdot \sqrt{\frac{2\ell_i + 1}{2} \frac{(\ell_i - |m_i|)!}{(\ell_i + |m_i|)!}} \cdot \sqrt{\frac{(k - |m_i - m_j|)!}{(k + |m_i + m_j|)!}} \cdot \sqrt{\frac{2\ell_j + 1}{2} \frac{(\ell_j - |m_j|)!}{(\ell_j + |m_j|)!}}$$

$$\cdot \int_0^\pi P_{\ell_i}^{|m_i|} P_k^{|m_i - m_j|} P_{\ell_j}^{|m_j|} \sin \theta d\theta$$

(15)

The integral in Eq. (15) is 0 if  $\ell_i$ ,  $k$  and  $\ell_j$  do not satisfy the inequalities and sum conditions for the sides of a triangle of even perimeter. If they do, we have

$$\int_0^\pi P_{\ell_i}^{|m_i|} P_k^{|m_i - m_j|} P_{\ell_j}^{|m_j|} \sin \theta d\theta =$$

$$2(-1)^{s-b-w} \frac{(h+v)!(s+w)!(2s-2s)! s!}{(h-v)!(s-\xi)!(s-b)!(s-s)!(2s+1)!}$$

$$\cdot \sum_{t=0}^{t=t_{\max}} (-1)^t \frac{(s+u+t)!(h+s-u-t)!}{t!(\xi-u-t)!(h-s+u+t)!(s-w-t)!}$$

(16)

where  $s = \frac{1}{2}(\ell_i + k + \ell_j)$ ,  $u$  is the largest of  $|m_i|$ ,  $|m_i - m_j|$  and  $|m_j|$ ,  $\xi$  is the subscript corresponding to  $u$ ,  $h$  is the larger of the two remaining subscripts,  $v$  is the superscript corresponding to  $h$ ,  $s$  is the remaining subscript,  $w$  is the remaining superscript, and  $t_{\max}$  is the smaller of  $s - w$  and  $\xi - u$ . The  $B$ 's in Eq. (13) have the form,

$$B(u, v, p, q) = \int_0^\infty \int_0^{h_1} e^{-u h_1 - v h_2} h_1^{p-1} h_2^{q-1} dh_2 dh_1 \quad (17)$$

For  $p \geq 0$ ,  $q \geq 0$ ,  $u \geq 0$  and  $v \geq 0$ , one has<sup>9</sup>

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<sup>9</sup> S.F. Boys, Proc. Roy. Soc. London, A 201, 125 (1950).

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$$B(u, v, p, q) = \sum_{\lambda=0}^p \frac{p! (p+q-\lambda)!}{(p-\lambda)!} \frac{1}{u^{1+\lambda}} \frac{1}{(u+v)^{p+q+1-\lambda}} \quad (18)$$

On the other hand, for  $p \leq -1$ ,  $q \geq |p|-1$ ,  $u \geq 0$ ,  $v \geq 0$ , one can show that

$$\begin{aligned} B(u, v, p, q) = & \frac{q!}{v^{q+1}} \left\{ (-1)^{|p|-1} \frac{u^{|p|-1}}{(|p|-1)!} \ln \frac{u+v}{u} + \right. \\ & + \sum_{k=1}^{|p|-1} (-1)^{k-1} \frac{v^{|p|-k} u^{k-1}}{(|p|-k) (|p|-1)!} \\ & \left. - \{1 - \delta(q, |p|-1)\} v^{|p|-1} \sum_{n=1}^{q-|p|+1} \frac{v^n (n-1)!}{(n+|p|-1)! (u+v)^n} \right\} \quad (19.1) \end{aligned}$$

or alternatively

$$B(u, v, p, q) = \frac{q!}{v^{q+1}} \sum_{\Delta=q+1}^{\infty} \frac{v^{\Delta} (\Delta-|p|)!}{\Delta! (u+v)^{\Delta-(|p|-1)}} \quad (19.2)$$

The  $\Delta$ 's are multiplied by products of Clebsch-Gordon coefficients,

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M.E. Rose, Angular Momentum (John Wiley and Sons, Inc., New York, 1957), p. 39.

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$$\begin{aligned}
C(\ell, \lambda, L, m) = & (-1)^{\lambda-m} L! \left\{ (2L+1) \frac{(\ell+\lambda-L)! (\ell-\lambda+L)! (-\ell+\lambda+L)!}{(\ell+\lambda+L+1)!} \right\}^{\frac{1}{2}} \\
& \cdot \frac{1}{[(\ell-m)! (\ell+m)! (\lambda-m)! (\lambda+m)!]^{\frac{1}{2}}} \\
& \cdot \sum_{\nu=\lambda-\ell}^L \frac{(-1)^\nu}{\nu!} \frac{(\lambda+L+m-\nu)! (\ell-m+\nu)!}{(-\ell+\lambda+L-\nu)! (L-\nu)! (\ell-\lambda+\nu)!}
\end{aligned} \quad (20)$$

where  $\ell \leq \lambda$ . Finally the spin factors must be taken into account.

The  $N_{ij}$ 's in Eq. (5), like the  $H_{ij}$ 's, will be a sum of four terms in the general case. If we again omit the Clebsch-Gordon coefficients, the normalization constant,  $N$ , and the spin factors, a typical member of these four terms will have the form

$$f = \frac{c_i c_j}{z^{x+y+2}} \delta(\ell_i, \ell_j) \delta(m_i, m_j) \delta(\lambda_i, \lambda_j) \frac{x!}{u^{x+1}} \frac{y!}{v^{y+1}} \quad (21)$$

Results

Table I gives the computed energies expressed in rydbergs for the various members of the  $1S$ ,  $3S$ ,  $1P$ ,  $3P$ ,  $1D$  and  $3D$  series. This table has been presented elsewhere<sup>5</sup> but is repeated here for completeness. The column headed  $\Delta E$  gives the difference

in millionths of a rydberg, that is, roughly in units of  $.1 \text{ cm}^{-1}$ , between the experimentally determined energies and those calculated in the present work. For the  $1^1S$ ,  $2^1S$  and  $2^3S$  the experimental values have been replaced by these values with the relativistic, radiative and ~~mass polarization~~ <sup>mass polarization</sup> effects as given by C.L. Pekeris removed.<sup>11</sup> The column headed  $\Delta E_p$  gives

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<sup>11</sup> C.L. Pekeris, Phys. Rev., 112, 1649 (1958), Phys. Rev., 115, 1216 (1959), Phys. Rev., 126, 1470 (1962).

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the similar difference between the experimental energies, or in the case of  $1^1S$ ,  $2^1S$  and  $2^3S$  the modified experimental values, and the energies found by C.L. Pekeris using the method of perimetric coordinates.

It appears from an examination of Table I that the present work reaches a rather substantial degree of accuracy in reproducing the observed energies. For the more highly excited states,

the energies found here are the lowest so far obtained by the minimum principle. It is to be expected that the wave function will improve as the difference between the observed and the calculated energy decreases. Unfortunately it is not clear that the improvement in the wave function proceeds at the same rate as the improvement in the energy representation.

In view of this uncertainty as to the quality of the wave functions and the sensitivity of the oscillator strengths to the precise form of the wave functions, which was mentioned above, it is very desirable to compute f-values from each of the three alternative expressions, that is, in terms of the dipole length, velocity, and acceleration.<sup>12</sup>

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<sup>12</sup> S. Chandrasekhar, *Astrophys. J.*, 102, 223 (1945).

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For two-electron systems, these expressions take the form<sup>13</sup>

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<sup>13</sup> B. Schiff and C.L. Pekeris, *Phys. Rev.*, 134, A638 (1964).

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$$f_L = 2(E_{m'} - E_m) \left| \int \psi_{m'}^* (z_1 + z_2) \psi_m d\tau \right|^2 \quad (22.1)$$

$$f_v = \frac{2}{E_{m'} - E_m} \left| \int \psi_{m'}^* \left( \frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2} \right) \psi_m d\tau \right|^2 \quad (22.2)$$

$$f_a = \frac{2}{(E_{m'} - E_m)^3} \left| Z \int \psi_{m'}^* \left( \frac{z_1}{\lambda_1^3} + \frac{z_2}{\lambda_2^3} \right) \psi_m d\tau \right|^2 \quad (22.3)$$

where atomic units are used throughout and Z is the atomic number.

If  $\psi_n$ 's which are exact solutions of a Schrödinger equation are substituted into these expressions, the three computed  $f$ -values will be the same. If the solutions are only approximate, the differences between the computed results should decrease as the accuracy of the wave functions increases. However, exact agreement of the three computed  $f$ -values insures the physical significance of the results only if the wave functions which are employed are solutions of a Schrödinger equation which adequately represents the physical problem. In the present case, the relativistic, radiative, and <sup>mass polarization</sup> ~~spin-orbit~~ ~~hyperfine~~ effects have been neglected, but these effects are probably small so that the extent of the agreement of the results from the three expressions for the oscillator strength can be taken as a measure of the degree of confidence which can be placed in their physical significance.

Table II gives the oscillator strengths for the  $1^1S-n^1P$  series of HeI as computed from the three expressions in Eq. (22). The first column specifies which of the three equations was employed. The second column gives the value of the principal quantum number of the series electron in the usual spectroscopic description of the series. Column three gives the results of the present work, column four the results found by Trefftz et al.,<sup>14</sup>

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<sup>14</sup>E. Trefftz, A. Schlüter, K.-H. Dettmar and K. Jorgens, Z. Astrophys. 44, 1(1957).

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column five the results of Schiff and Pekeris<sup>13</sup> and column six the results for hydrogen as quoted by Bethe and Salpeter,<sup>15</sup>

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<sup>15</sup> H.A. Bethe and E.E. Salpeter, Handbuch der Physik, (Springer-Verlag, Berlin, 1957), Vol. 35, p. 351.

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from the work of Harriman<sup>16</sup>

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<sup>16</sup> J.M. Harriman, Phys. Rev., 101, 594 (1956).

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and as computed from the matrix elements given by Green et al.<sup>17</sup>

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<sup>17</sup> L.C. Green, P.P. Rush and C.D. Chandler, Astrophys. J. Supplement Series 3, 37 (1957).

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Perhaps the most encouraging aspect of Table II from the point of view of the present work is the fact that the oscillator strengths computed from the dipole acceleration expression are in reasonably good agreement with the results from the other two expressions. Experience in the past<sup>2,18</sup>

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<sup>18</sup> A.W. Weiss, Astrophys. J., 138, 1262 (1963).

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has largely shown that the length and velocity expressions, which weight the wave function more heavily at large and intermediate nuclear distances respectively, are in general in much better agreement with one another than with the acceleration expression which weights the wave function more heavily at small nuclear distances.

The acceleration expression may in fact differ by more than an order of magnitude from the other two. Chandrasekhar<sup>12</sup> pointed out long ago that the main contribution to the energy integral comes from intermediate nuclear distances so that the use of the minimum principle determines the wave function best in this region.

In summary, the agreement between the computed and experimental energies given in Table I, the agreement shown in Table II between the oscillator strengths as computed by the length, velocity, and acceleration expressions in the present work and the agreement between the present work and the very extensive computations of Schiff and Pekeris for the transitions  $1^1S-2^1P$  and  $1^1S-3^1P$  make it clear that, at least for two-electron systems, the use of central field functions and configuration interaction can give results of substantial accuracy. It seems therefore that this method deserves further exploration. In the course of this investigation, a number of wave functions of rather high accuracy have been found for various excited states of He I and oscillator strengths for a number of transitions in the  $1^1S-n^1P$  series have been obtained.

Table I. Energies of HeI in Rydbergs

n	$n^1S$			$n^3S$			$n^1P$		
	E	$\Delta E$	$\Delta E_p$	E	$\Delta E$	$\Delta E_p$	E	$\Delta E$	$\Delta E_p$
1	-5.806765	-684	-0						
2	-4.291875	-74	-13	-4.350427	-32	0	-4.247563	-116	+4
3	-4.122519	-26	-33	-4.137365	-13	0	-4.110250	-41	-16
4	-4.067164	-10	-48	-4.073016	-10	-2	-4.062118	-21	
5	-4.042348	-6	-53	-4.045233	-6	-2	-4.039800	-11	
6	-4.029122	-4	-55	-4.030752	-4	-5	-4.027661	-7	
7	-4.021249	-3	-52	-4.022258	-2	-12	-4.020334	-5	
8	-4.016186	0	-50	-4.016853	-2	-27	-4.015575	-4	
9	-4.012738	-2	-53	-4.013202	-2	-52			

n	$n^3P$			$n^1D$		$n^3D$	
	E	$\Delta E$	$\Delta E_p$	E	$\Delta E$	E	$\Delta E$
1							
2	-4.266256	-86	-15				
3	-4.116135	-31	-23	-4.111167	-76	-4.111213	-60
4	-4.064633	-18		-4.062523	-38	-4.062550	-28
5	-4.041092	-11		-4.040012	-21	-4.040027	-15
6	-4.028411	-4		-4.027784	-13	-4.027794	-9
7	-4.020806	-4		-4.020412	-10	-4.020419	-5
8	-4.015892	-2		-4.015628	-5	-4.015632	-4
9							

$\Delta E$  and  $\Delta E_p$  give the difference in millionths of a rydberg between the experimental energies and the values computed by the present authors and by Pekeris respectively. For the  $1^1S$ ,  $2^1S$ ,  $2^3S$  and  $3^3S$  terms, the relativistic, radiative, and mass polarization corrections have been applied to the experimental values.

Table II. Oscillator Strengths for the  $1^1S-n^1P$   
Series of HeI according to the Length,  
Velocity and Acceleration Expression

	n	Present Work	Trefftz et al.	Schiff and Pekeris	Hydrogen
Len.	2	.2701	.3113	.2761	.4162
Vel.		.2752	.2719	.2762	
Acc.		.2682		.2760	
Len.	3	.0734	.0824	.0736	.0791
Vel.		.0728	.0720	.0734	
Acc.		.0702		.0732	
Len.	4	.0299	.0303		.0290
Vel.		.0295	.0274		
Acc.		.0282			
Len.	5	.0151			.0139
Vel.		.0148			
Acc.		.0141			
Len.	6	.00863	.00800		.00780
Vel.		850	.00793		
Acc.		813			
Len.	7	.00541			.00481
Vel.		532			
Acc.		509			
Len.	8	.00361			.00318
Vel.		355			
Acc.		340			